

The Computational Complexity of Linear Optics

We give new evidence that quantum computers—moreover, rudimentary quantum computers built entirely out of linear-optical elements—cannot be efficiently simulated by classical computers. In particular, we define a model of computation in which identical photons are generated, sent through a linear-optical network, then nonadaptively measured to count the number of photons in each mode. This model is not known or believed to be universal for quantum computation, and indeed, we discuss the prospects for realizing the model using current technology. On the other hand, we prove that the model is able to solve sampling problems and search problems that are classically intractable under plausible assumptions. Our first result says that, if there exists a polynomial-time classical algorithm that samples from the same probability distribution as a linear-optical network, then $P^{\#P} = BPP^{NP}$, and hence the polynomial hierarchy collapses to the third level. Unfortunately, this result assumes an extremely accurate simulation. Our main result suggests that even an approximate or noisy classical simulation would already imply a collapse of the polynomial hierarchy. For this, we need two unproven conjectures: the *Permanent-of-Gaussians Conjecture*, which says that it is $\#P$ -hard to approximate the permanent of a matrix A of independent $\mathcal{N}(0, 1)$ Gaussian entries, with high probability over A ; and the *Permanent Anti-Concentration Conjecture*, which says that $|\text{Per}(A)| \geq \sqrt{n!}/\text{poly}(n)$ with high probability over A . We present evidence for these conjectures, both of which seem interesting even apart from our application. This paper does not assume knowledge of quantum optics. Indeed, part of its goal is to develop the beautiful theory of noninteracting bosons underlying our model, and its connection to the permanent function, in a self-contained way accessible to theoretical computer scientists.

Quantum algorithm for solving linear systems of equations

Solving linear systems of equations is a common problem that arises both on its own and as a subroutine in more complex problems: given a matrix A and a vector b , find a vector x such that $Ax=b$. We consider the case where one doesn't need to know the solution x itself, but rather an approximation of the expectation value of some operator associated with x , e.g., $x'Mx$ for some matrix M . In this case, when A is sparse, N by N and has condition number κ , classical algorithms can find x and estimate $x'Mx$ in $O(N \sqrt{\kappa})$ time. Here, we exhibit a quantum algorithm for this task that runs in $\text{poly}(\log N, \kappa)$ time, an exponential improvement over the best classical algorithm.

Identifying folding nucleus based on residue contact networks of proteins

In the native structure of a protein, all the residues are tightly parked together in a specific order following its folding and every residue contacts with some spatially neighbor residues. A residue contact network can be constructed by defining the residues as nodes and the native contacts as edges. During the folding of small single-domain proteins, there is a set of contacts (or bonds), defined as the folding nucleus (FN), which is formed around the transition state, i.e., a rate-limiting barrier located at about the middle between the unfolded states and the native state on the free energy landscape. Such a FN plays an essential role in the folding dynamics and the residues, which form the related contacts called as folding nucleus residues (FNRs). In this work, the FNRs in proteins are identified by using quantities which characterize the topology of residue contact networks of proteins. By comparing the specificities of residues with the network quantities KR , LR , and DR , up to 90% FNRs of six typical proteins found experimentally are identified. It is found that the FNRs behave the full-closeness centrals rather than degree or closeness centers in the residue contact network, implying that they are important to the folding cooperativity of proteins. Our study shows that the FNRs can be identified solely from the native structures of proteins based on the analysis of residue contact network without any knowledge of the transition state ensemble.

Frustration, specific sequence dependence, and nonlinearity in large-amplitude fluctuations of allosteric proteins

Proteins have often evolved sequences so as to acquire the ability for regulation via allosteric conformational change. Here we investigate how allosteric dynamics is designed through sequences with nonlinear interaction features. First, for 71 allosteric proteins of which two, open and closed, structures are available, a statistical survey of interactions using an all-atom model with effective solvation shows that those residue contact interactions specific to one of the two states are significantly weaker than are the contact interactions shared by the two states. This interaction feature indicates there is underlying sequence design to facilitate conformational change. Second, based on the energy landscape theory, we implement these interaction features into a new atomic-interaction-based coarse-grained model via a multiscale simulation protocol (AICG). The AICG model outperforms standard coarse-grained models for predictions of the native-state mean fluctuations and of the conformational change direction. Third, using the new model for adenylate kinase, we show that intrinsic fluctuations in one state contain rare and large-amplitude motions nearly reaching the other state. Such large-amplitude motions are realized partly by sequence specificity and partly by the nonlinear nature of contact interactions, leading to cracking. Both features enhance conformational transition rates.

[Chiral spin states and superconductivity]

It is shown that several different order parameters can be used to characterize a type of P- and T-violating state for spin systems, that we call chiral-spin states. There is a closely related, precise notion of chiral-spin-liquid states. We construct soluble models, based on P- and T-symmetric local-spin Hamiltonians, with chiral-spin ground states. Mean-field theories leading to chiral spin liquids are proposed. Frustration is essential in stabilizing these states. The quantum numbers of quasiparticles around the chiral spin liquids are analyzed. They generally obey fractional statistics. Based on these ideas, it is speculated that superconducting states with unusual values of the flux quantum may exist.

[Charged boson condensation in high-temperature superconductors]

We explore the superconducting transition in the RVB (resonant valence bond) model, assuming that the superconductivity is due to a Bose-Einstein condensation of charged bosons in the RVB vacuum. It appears that the charged bosons behave like a weakly interacting $2 + \epsilon$ dimensional boson gas and that the RVB superconductors exhibit many two-dimensional properties. Among others are a linear temperature dependence of the critical fields, which has already been observed in experiments, and a linear doping dependence of the transition temperature.

Particle Creation by Black Holes

Abstract. In the classical theory black holes can only absorb and not emit particles. However it is shown that quantum mechanical effects cause black holes to create and emit particles as if they were hot bodies with temperature $\frac{\hbar\kappa}{2\pi k} \approx 10^{-6} \left(\frac{M_{\odot}}{M}\right) ^{\circ}\text{K}$ where κ is the surface gravity of the black hole. This thermal emission leads to a slow decrease in the mass of the black hole and to its eventual disappearance: any primordial black hole of mass less than about 10^{15} g would have evaporated by now. Although these quantum effects violate the classical law that the area of the event horizon of a black hole cannot decrease, there remains a Generalized Second Law: $S + \frac{1}{4}A$ never decreases where S is the entropy of matter outside black holes and A is the sum of the surface areas of the event horizons. This shows that gravitational collapse converts the baryons and leptons in the collapsing body into entropy. It is tempting to speculate that this might be the reason why the Universe contains so much entropy per baryon.

Quantum Computation vs. Firewalls

ABSTRACT: In this paper we discuss quantum computational restrictions on the types of thought experiments recently used by Almheiri, Marolf, Polchinski, and Sully to argue against the smoothness of black hole horizons. We argue that the quantum computations required to do these experiments would take a time which is exponential in the entropy of the black hole under study, and we show that for a wide variety of black holes this prevents the experiments from being done. We interpret our results as motivating a broader type of nonlocality than is usually considered in the context of black hole thought experiments, and claim that once this type of nonlocality is allowed there may be no need for firewalls. Our results do not threaten the unitarity of black hole evaporation or the ability of advanced civilizations to test it.

Rotation Forest: A New Classifier Ensemble Method

We propose a method for generating classifier ensembles based on feature extraction. To create the training data for a base classifier, the feature set is randomly split into K subsets (K is a parameter of the algorithm) and principal component analysis (PCA) is applied to each subset. All principal components are retained in order to preserve the variability information in the data. Thus, K axis rotations take place to form the new features for a base classifier. The idea of the rotation approach is to encourage simultaneously individual accuracy and diversity within the ensemble. Diversity is promoted through the feature extraction for each base classifier. Decision trees were chosen here because they are sensitive to rotation of the feature axes, hence the name "forest". Accuracy is sought by keeping all principal components and also using the whole data set to train each base classifier. Using WEKA, we examined the rotation forest ensemble on a random selection of 33 benchmark data sets from the UCI repository and compared it with bagging, AdaBoost, and random forest. The results were favorable to rotation forest and prompted an investigation into diversity-accuracy landscape of the ensemble models. Diversity-error diagrams revealed that rotation forest ensembles construct individual classifiers which are more accurate than these in AdaBoost and random forest, and more diverse than these in bagging, sometimes more accurate as well

Random Forest

Random forests are a combination of tree predictors such that each tree depends on the values of a random vector sampled independently and with the same distribution for all trees in the forest. The generalization error for forests converges a.s. to a limit as the number of trees in the forest becomes large. The generalization error of a forest of tree classifiers depends on the strength of the individual trees in the forest and the correlation between them. Using a random selection of features to split each node yields error rates that compare favorably to Adaboost, but are more robust with respect to noise. Internal estimates monitor error, strength, and correlation and these are used to show the response to increasing the number of features used in the splitting. Internal estimates are also used to measure variable importance. These ideas are also applicable to regression.